COMPUTING PROCEDURES FOR ESTIMATING VARIANCE COMPONENTS FROM UNBALANCED DATA IN THE 2-WAY CROSSED CLASSIFICATION, NO INTERACTION, MIXED MODEL

BU-450-M by September, 1973

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Abstract

Available methods for estimating variance components from unbalanced data in mixed models yield specific computing formulae for the 2-way crossed classification without interaction.

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Summary

Available methods for estimating variance components from unbalanced data in mixed models yield specific computing formulae for the 2-way crossed classification without interaction.

1. Introduction

The easiest method for estimating variance components from unbalanced data is the analysis of variance method, Henderson's [1953] Method 1. However, it is seldom used with mixed models because it then yields biased estimators. Several other methods are available, of which three are considered here: the fitting constants method (Henderson's Method 3), an iterative method based on Thompson [1969], and Henderson's Method 2. Each of these is applied to the model

$$y_{ijk} = \mu + \alpha_i + \beta_j + e_{ijk} \tag{1}$$

with $i = 1, \cdots, a$, $j = 1, \cdots, b$ and $k = 1, \cdots, n_{ij}$ with the α's being random effects (with zero mean and variance σ_α^2) and the β's being fixed effects. Since in most data for which this might be a reasonable model the number of fixed effects will be considerably less than the number of random effects we assume $b < a$, noting that often we will have $b \ll a$.

Two of the methods considered here, the fitting constants and the iterative methods, are discussed in some detail in Searle [1971]. The other, Henderson's

Method 2, has since been shown by Henderson et al. [1973] to be a validly defined procedure and so is available for use with model (1). Only the application of the methods to model (1) is given here. Their general development is available elsewhere (see references). In developing the computing formulae for (1) repeated use is made of Searle [1971], hereafter referred to as LM, and the same notation is used here as there.

2. Fitting constants estimators

For the sake of completeness we repeat the fitting constants estimators given in LM p. 490.

$$T_o = \Sigma\Sigma\Sigma y_{ijk}^2$$

$$T_B = \sum \frac{y_{\cdot j \cdot}^2}{n_{\cdot j}} \qquad T_A = \sum \frac{y_{i \cdot \cdot}^2}{n_{i \cdot}}$$

$R(\mu,\alpha,\beta) = T_A + t_B$, as on LM p. 484

$h_7 = N - k_4 = N - \sum_j \frac{\Sigma_i n_{ij}^2}{n_{i\cdot}}$, as on LM p. 480 and 488

$$\hat{\sigma}_e^2 = \frac{T_o - R(\mu,\alpha,\beta)}{N - a - b + 1}$$

$\hat{\sigma}_\alpha^2 = \dfrac{R(\mu,\alpha,\beta) - T_B - (a - 1)\hat{\sigma}_e^2}{h_7}$, as on LM p. 490.

Note that it is immaterial to the calculation of $R(\mu,\alpha,\beta)$ whether it is the α's or the β's that are defined as the fixed effects. However, having decided to define β's as fixed effects and concluded that $b < a$ as a consequence, the easiest calculation of $R(\mu,\alpha,\beta)$ will then be that shown on LM p. 484, as derived in equation (26) on p. 270.

3. Iterative estimators

An iterative procedure for models having one random factor is outlined in Sec. 11.7c on p. 490 of LM. It stems from equations (146) and (147) on p. 469, and its application to the model (1) is as follows.

With the elements of $\underline{y}$ ordered j within i in the usual manner we have (1) as

$$\underline{y} = \mu \underline{1}_N + \underline{Z}\underline{\alpha} + \underline{X}\underline{\beta} + \underline{e} \quad .$$

On defining

$$\underline{b} = \{b_j\} = \{\mu + \beta_j\} \text{ for } j = 1 \cdots b \;,$$

and $$\underline{u} = \underline{\alpha}$$

we then have

$$\underline{Y} = \underline{X}\underline{b} + \underline{Z}\underline{u} + \underline{e} \tag{2}$$

where $\underline{X}$ = design matrix, order $N \times b$, for the β_j-effects

and $$\underline{Z} = \sum_{i=1}^{a}{}^{+} \underline{1}_{n_{i.}} \quad .$$

Example

$$n_{ij} = \begin{array}{ccc|c} 2 & 1 & 0 & 3 \\ 1 & 1 & 1 & 3 \\ \hline 3 & 2 & 1 & 6 \end{array} \qquad \underline{X} = \begin{bmatrix} 1 & . & . \\ 1 & . & . \\ . & 1 & . \\ 1 & . & . \\ . & 1 & . \\ . & . & 1 \end{bmatrix} \qquad \underline{Z} = \begin{bmatrix} 1 & . \\ 1 & . \\ 1 & . \\ . & 1 \\ . & 1 \\ . & 1 \end{bmatrix} .$$

In general, $\underset{\sim}{X}$ can be written as

$$\underset{\sim}{X} = \begin{bmatrix} \Sigma^*_j \ \underset{\sim}{1}_{n_{1j}} \\ \Sigma^*_j \ \underset{\sim}{1}_{n_{2j}} \\ \vdots \\ \Sigma^*_j \ \underset{\sim}{1}_{n_{aj}} \end{bmatrix} = \left\{ \Sigma^*_j \ \underset{\sim}{1}_{n_{ij}} \right\} \quad \text{for } i = 1, 2, \cdots, a$$

where $\Sigma^*_j \ \underset{\sim}{1}_{n_{ij}}$ is a matrix of b columns and is a direct sum of vectors $\underset{\sim}{1}_{n_{ij}}$, but with the convention that the t'th column is "skipped" when $n_{it} = 0$, and so is null. For example, with

$$n_{ij} = 2,0,4,3,0,6$$

$$\Sigma^*_j \ \underset{\sim}{1}_{n_{1j}} = \begin{bmatrix} \underset{\sim}{1}_2 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \underset{\sim}{1}_4 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \underset{\sim}{1}_3 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \underset{\sim}{1}_6 \end{bmatrix} .$$

This is a slight deviation from the notation Σ^+ for familiar direct sums.

For $\underset{\sim}{X}$ and $\underset{\sim}{Z}$ as now defined we then have

$$\underset{\sim}{X}'\underset{\sim}{X} = \underset{\sim}{D}\{n_{.j}\} \quad \text{for } j = 1 \cdots b ,$$

where $\underset{\sim}{D}\{\ \}$ denotes a diagonal matrix, in this case of the $n_{.j}$'s; and

$$\underset{\sim}{Z}'\underset{\sim}{X} = \{n_{ij}\} \quad \text{for } i = 1 \cdots a \text{ and } j = 1 \cdots b ,$$

$$\underset{\sim}{Z}'\underset{\sim}{Z} = \underset{\sim}{D}\{n_{i.}\}$$

Derivation of calculations

The starting point is LM pages 489-90.

$$r = r(\underset{\sim}{X}) = b$$

$$\begin{aligned} c &= \operatorname{tr}\left[\underset{\sim}{Z}'\underset{\sim}{Z} - \underset{\sim}{Z}'\underset{\sim}{X}(\underset{\sim}{X}'\underset{\sim}{X})^{-}\underset{\sim}{X}'\underset{\sim}{Z}\right] \\ &= \operatorname{tr}\left(\underset{\sim}{D}\{n_{i.}\} - \{n_{ij}\}D\{1/n_{.j}\}\{n_{ij}\}'\right) \\ &= \sum_i n_{i.} - \operatorname{tr}\left(\{n_{ij}/n_{.j}\}\{n_{ij}\}'\right) \\ &= N - \sum_{ij}\sum n_{ij}^2/n_{.j} = N - \sum_j \frac{1}{n_{.j}} \sum n_{ij}^2 \\ &= N - k_4, \text{ using LM p. 480} \\ &= h_7, \text{ as on LM p. 488.} \end{aligned}$$

For the example

$$\underset{\sim}{Z}'\underset{\sim}{X}(\underset{\sim}{X}'\underset{\sim}{X})^{-1}\underset{\sim}{X}'\underset{\sim}{Z} = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{3} & \cdot & \cdot \\ \cdot & \frac{1}{2} & \cdot \\ \cdot & \cdot & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 \\ 1 & 1 \\ 0 & 1 \end{bmatrix}$$

for which the trace is $2^2/3 + 1^2/2 + 1^2/1 = k_4$ as above.

Since $\underset{\sim}{Z}'\underset{\sim}{Z} = \underset{\sim}{D}\{n_{i.}\}$ and with $\lambda = \sigma_e^2/\sigma_\alpha^2$ we have

$$\underset{\sim}{P} = \underset{\sim}{Z}'\underset{\sim}{Z} + \lambda\underset{\sim}{I} = \underset{\sim}{D}\{n_{i.} + \lambda\} \qquad \text{for } i = 1, \cdots, a$$

and so with

$$\begin{aligned} \underset{\sim}{T} &= \underset{\sim}{I} - \underset{\sim}{Z}\underset{\sim}{P}^{-1}\underset{\sim}{Z}' \\ \underset{\sim}{T}\underset{\sim}{y} &= \underset{\sim}{y} - \underset{\sim}{Z}\underset{\sim}{P}^{-1}\underset{\sim}{Z}'\underset{\sim}{y} = \underset{\sim}{y} - \underset{\sim}{Z}\underset{\sim}{P}^{-1}\{y_{i..}\} \quad i = 1, \cdots, a \\ &= \underset{\sim}{y} - \underset{\sim}{Z}\left\{\frac{y_{i..}}{n_{i.} + \lambda}\right\} \end{aligned}$$

$$= \left\{y_{ijk} - \frac{y_{i..}}{n_{i.} + \lambda}\right\} \text{for } i = 1, \cdots, a,\ j = 1, \cdots, b$$

and $k = 1, \cdots, n_{ij}$, in lexicon order ,

$$\underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{y} = \left\{y_{.j.} - \sum_i \frac{n_{ij}y_{i..}}{n_{i.} + \lambda}\right\} \quad \text{for } j = 1, \cdots, b \quad .$$

When $\lambda = 0$ the elements of $\underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{y}$ are r_j for $j = 1, \cdots, b$, the first $b - 1$ of which constitute $\underset{\sim}{r}$ on LM p. 484.

We now need

$$R^*(\underset{\sim}{b}|\underset{\sim}{u}) = R^*(\mu,\beta|\alpha) = \underset{\sim}{y}'\underset{\sim}{T}\underset{\sim}{X}(\underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{X})^-\underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{y} \quad .$$

Note the misprint in this expression in LM p. 490: $(\underset{\sim}{X}\underset{\sim}{T}\underset{\sim}{X}')^-$ should be $(\underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{X})^-$. From the above expressions we have

$$\underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{X} = \underset{\sim}{X}'\underset{\sim}{X} - \underset{\sim}{X}'\underset{\sim}{Z}\underset{\sim}{P}^{-1}\underset{\sim}{Z}'\underset{\sim}{X} = \underset{\sim}{D}\{n_{.j}\} - \underset{\sim}{X}'\underset{\sim}{Z}\underset{\sim}{P}^{-1}\underset{\sim}{Z}'\underset{\sim}{X} \quad \text{for } j = 1, \cdots, b$$

and

$$\underset{\sim}{P}^{-1}\underset{\sim}{Z}'\underset{\sim}{X} = \underset{\sim}{D}\{1/(n_{.j} + \lambda)\}\{n_{ij}\} = \left\{\frac{n_{ij}}{n_{i.} + \lambda}\right\} \quad \text{for } i=1,\cdots,a \text{ and } j=1,\cdots,b \quad .$$

Hence

$$\underset{\sim}{X}'\underset{\sim}{Z}\underset{\sim}{P}^{-1}\underset{\sim}{Z}'\underset{\sim}{X} = \left\{\sum_i \frac{n_{ij}n_{ij'}}{n_{i.} + \lambda}\right\} \quad \text{for } j,j' = 1,\cdots,b$$

and so

$$\underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{X} = \underset{\sim}{D}\{n_{.j}\} - \left\{\sum_i \frac{n_{ij}n_{ij'}}{n_{i.} + \lambda}\right\} \quad \text{for } j,j' = 1,\cdots,b \quad .$$

When $\lambda = 0$, the leading sub-matrix of order $(b - 1) \times (b - 1)$ in $\underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{X}$ is $\underset{\sim}{C}$ on p. 484 of LM.

On now defining

$$\underset{\sim}{C}_* = \underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{X} = \underset{\sim}{D}\{n_{.j}\} - \left\{\sum_i \frac{n_{ij}n_{ij'}}{n_{i.} + \lambda}\right\} \quad \text{for } j,j' = 1,\cdots,b$$

and

$$\underset{\sim}{r}_* = \underset{\sim}{X}'\underset{\sim}{T}\underset{\sim}{y} = \left\{y_{.j.} - \sum_i \frac{n_{ij}y_{i..}}{n_{i.} + \lambda}\right\} \quad \text{for } j = 1,\cdots,b$$

we therefore have

$$R^*(\underset{\sim}{b}|\underset{\sim}{u}) = \underset{\sim}{r}_*'\underset{\sim}{C}_*^{-1}\underset{\sim}{r}_*$$

analogous to the form $\underset{\sim}{r}'\underset{\sim}{C}^{-1}\underset{\sim}{r}$ on LM p. 484. (Note, however, that $\underset{\sim}{C}$ has order $b - 1$ whereas $\underset{\sim}{C}_*$ has order b).

We also have

$$R^*(\underset{\sim}{u}) = R^*(\alpha) = \underset{\sim}{y}'\underset{\sim}{Z}\underset{\sim}{P}^{-1}\underset{\sim}{Z}'\underset{\sim}{y} = \sum_i \frac{y_{i..}^2}{n_{i.} + \lambda}$$

and

$$R^*(b) = R(\mu,\beta) = \sum_j \frac{y_{.j.}^2}{n_{.j}} = T_B \quad .$$

The calculations are therefore as follows.

Calculations

$\lambda = 1$ (or some other value assigned by the user)

$$\underset{\sim}{C}_*^{-1} = \{c_*^{jj'}\} = \left(\underset{\sim}{D}\{n_{.j}\} - \left\{\sum_i \frac{n_{ij}n_{ij'}}{n_{i.} + \lambda}\right\}\right)^{-1} \quad \text{for } j,j' = 1,\cdots,b$$

$$R^*(\mu,\beta|\alpha) = \sum_j c_*^{jj}\left(y_{.j.} - \sum_i \frac{n_{ij}y_{i..}}{n_{i.} + \lambda}\right)^2 + 2\sum_{j<j'}\sum c_*^{jj'}\left(y_{.j.} - \sum_i \frac{n_{ij}y_{i..}}{n_{i.} + \lambda}\right)\left(y_{.j'.} - \sum_i \frac{n_{ij'}y_{i..}}{n_{i.} + \lambda}\right)$$

$$R^*(\mu,\alpha,\beta) = R^*(\mu,\beta|\alpha) + \sum_i \frac{y_{i..}^2}{n_{i.} + \lambda}$$

$$R^*(\alpha|\mu,\beta) = R^*(\mu,\alpha,\beta) - T_B$$

$$\tilde{\sigma}_e^2 = \frac{T_o - R^*(\mu,\alpha,\beta)}{N - b}$$

$$\tilde{\sigma}_\alpha^2 = \frac{R^*(\alpha|\mu,\beta)}{h_7}$$

Now, with

$$\tilde{\lambda} = \frac{\tilde{\sigma}_e^2}{\tilde{\sigma}_\alpha^2},$$

repeat until successive values of $\tilde{\lambda}$ are equal to within some tolerance, say 0.1 or 0.01.

4. Method 2 estimators

A recent summary of Method 2 is given in Henderson *et al.* [1973]. In terms of a general model

$$\underline{y} = \underline{X}\underline{\beta} + \underline{Z}\underline{u} + \underline{e} \tag{3}$$

where $\underline{\beta}$ represents the fixed effects and $\underline{u}$ the random effects the method involves solving

$$\begin{bmatrix} \underline{X}'\underline{X} & \underline{X}'\underline{Z} \\ \underline{Z}'\underline{X} & \underline{Z}'\underline{Z} \end{bmatrix} \begin{bmatrix} \underline{\beta}^o \\ \underline{u}^o \end{bmatrix} = \begin{bmatrix} \underline{X}'\underline{y} \\ \underline{Z}'\underline{y} \end{bmatrix} \tag{4}$$